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Comprehensive two-dimensional gas chromatography (GC × GC) measurements of volatile organic compounds in the atmosphere

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Abstract. During the MINOS campaign in August 2001 comprehensive twodimensional gas chromatography (GC x GC) was applied to the in situ measurements of atmospheric volatile organic compounds (VOCs) at the Finokalia ground station, Crete. The measurement system employs a thermal desorption unit for on-line sampling and injection, and a GC x GC separation system equipped with a flame ionization detector (FID) for detection. The system was optimized to resolve C₇-C₁₄ organic components. Two-dimensional chromatograms from measurements of Finokalia air samples show several hundred well-separated peaks. To facilitate peak identification, cartridge samples collected at Finokalia were analyzed using the same GC x GC system coupled with a time-of-flight mass spectrometer (TOF-MS). The resulting mass spectra were deconvoluted and compared to spectra from a database for tentative peak identification. About 650 peaks have been identified in the two-dimensional plane, with significant signal/noise ratios (>100) and high spectra similarities (>800). By comparing observed retention indices with those found in the literature, 235 of the identifications have been confirmed. 150 of the confirmed compounds show up in the C₇-C_{1,4} range of the chromatogram from the in situ measurement. However, at least as many peaks remain unidentified. For quantification of the GC x GC measurements, peak volumes of measured compounds have been integrated and externally calibrated using a standard gas mixture.

■ Final Revised Paper (PDF, 349 KB)
■ Discussion Paper (ACPD)

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